# NANOSCALE MODELING AND SIMULATION

Small Group Initiative

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## *Program Solicitation*

## *NSF 00-36*

DIRECTORATE FOR ENGINEERING

***DEADLINE DATE: APRIL 10, 2000***


NATIONAL SCIENCE FOUNDATION


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# SUMMARY OF PROGRAM REQUIREMENTS

## GENERAL INFORMATION

**Program Name:** Nanoscale Modeling and Simulation – Small Group Initiative

**Short Description/Synopsis of Program:**

The Division of Engineering Education and Centers, in collaboration with the other divisions in the Directorate for Engineering, announces a small-group (3-5 researchers each) initiative on research in engineering modeling and simulation at the nanoscale, with a focus on transdisciplinary research among various disciplines (physics, chemistry, biology, material science, engineering, thermodynamics, mechanics, electronics, and others) and areas of nanoscale relevance (nanostructured materials, nanodevices, large surface area structures, optoelectronics, synthesis, processing and manufacturing, instrumentation, environment, and others). Currently, modeling at the nanoscale is generally constrained at the level of single phenomenon and small systems. However, it is critical to consider the interplay of coupled and time-dependent phenomena in larger atomistic and molecular systems. The purpose of this initiative is to develop a knowledge base of the interplay of multiphenomena at multiscales by encouraging synergistic interaction among research groups with different areas of interest in nanoscale modeling and simulation. The goal is to support three to five groups, each focusing on a set of coupled phenomena over a few length scales and a set of methodologies. The intent of the overall initiative is to support an assemblage of groups that cover a broad range of phenomena and processes in key areas. NSF expects that a synergistic relationship among the funded groups will develop over time. Funded groups will be selected to span a complementary range of disciplines and methodologies.

**Cognizant Program Officers:**


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Cheryl Cathey, ccathey@nsf.gov; or Lynn Preston, lpreston@nsf.gov, 703-306-1380
Division of Engineering Education and Centers
This Division will receive the proposals, manage the review process, and administer the awards. (Proposers are reminded to identify the program solicitation number (NSF 00-36) in the program announcement/solicitation block on the Cover Sheet.)

**Applicable Catalog of Federal Domestic Assistance (CFDA) No.:** 47.041 — Engineering Grants

## ELIGIBILITY

- Limitation on the categories of organizations that are eligible to submit proposals:

  **Proposals must be submitted by U.S. academic institutions with undergraduate and Ph.D. programs.**

- PI eligibility limitations:

  **Open to small groups of three to five investigators.**

- Limitation on the number of proposals that may be submitted by an organization:

  **An institution (university or campus of a multi-campus university) may submit one proposal where only researchers from that institution are involved. The same institution may also submit one other proposal as the lead institution in a multi-institution group proposal. That same institution may be a partner in any number of other multi-university group proposals in which it is not the lead.**

## AWARD INFORMATION

- Type of award anticipated:

  **Awards will be standard or continuing grants for $300,000 to $700,000 per year, depending upon the number of investigators and the nature of the research activity, with duration of up to three years.**

- Number of awards anticipated in FY 00: **3-5 awards.**

- Amount of funds available: **Approximately $3 million will be available for this initiative in FY 2000.**

- Anticipated date of award: **September 2000.**

## PROPOSAL PREPARATION & SUBMISSION INSTRUCTIONS

- **Proposal Preparation Instructions**

- Letter of Intent requirements: **None.**
- Preproposal requirements: **None.**
- Proposal preparation instructions:

  **Standard NSF Grant Proposal Guide instructions (NSF 00-2).**
- Supplemental proposal preparation instructions:

  **The plan for industry/university collaboration must be presented in the proposal.**
- Deviations from standard (GPG) proposal preparation instructions: **None.**

♦ **Budgetary Information**

- Cost sharing/matching requirements: **None.**
- Indirect cost (F&A) limitations: **None.**
- Other budgetary limitations: **None.**

♦ **FastLane Requirements**

- FastLane proposal preparation requirements: **FastLane use required.**
- FastLane point of contact**:**

  **Esther Bolding,** ebolding@nsf.gov**, (703) 306-1380.**

♦ **DEADLINE/TARGET DATES**

- Proposal Deadline: **5:00 PM your local time, April 10, 2000 (FastLane).**

**PROPOSAL REVIEW INFORMATION**

♦ **The standard National Science Board approved criteria will be used to review the proposals, plus the criteria below:**
- **The level of expertise and accomplishment of the proposers in a discipline or field of relevance to modeling and simulation at the nanoscale;**
- **The potential of the proposed activity to enhance the interplay of multiphenomena at multiscales in different areas of nanoscale modeling and simulation;**

- **The degree to which the proposed activity will stimulate cross-disciplinary education through the development of curricula and the involvement of students in the research;**
- **The level of involvement of undergraduate and graduate students in the research; and**
- **The strength of the plans for the required collaboration with industry.**

## AWARD ADMINISTRATION INFORMATION

- Grant Award Conditions: **GC-1 or FDP III.**
- Special grant conditions anticipated: **None anticipated.**
- Special reporting requirements anticipated: **None.**

## I. INTRODUCTION

Nanotechnology arises from the exploitation of physical, chemical and biological properties of systems that are intermediate in size between isolated atoms/molecules and bulk materials, where phenomena length scales become comparable to the size of the structure. The discovery of novel properties, phenomena and processes at the 'nano' scale, from about 1 to 100 nm, and the development of new experimental and theoretical tools in the last few years for investigating these structures, provides fresh opportunities for scientific and technology developments in nanoparticles, nanostructured materials and nanodevices. A critical issue for nanotechnology is the ability to understand, model and simulate the behavior of the small structures and to make the connection between structure, properties and functions. Most nanosystems are too small for direct measurements, too large to be described by current rigorous first principles in theoretical and in computational methods, exhibit too many fluctuations to be treated monolithically in time and space, and are too few to be described by a statistical ensemble (see Chapter 2 of the publication "Nanotechnology Research Directions, IWGN Workshop Report," NSTC, 1999, on the website http://www.nsf.gov/nano).

Modeling and simulation methods at the nanoscale have originated from separate work in various disciplines and areas of relevance, but have arrived at the same time at the atomistic and molecular levels with, at times, similar governing equations. However, research efforts in nanoscale science and engineering are still relatively fragmented. More realistic simulations are needed to address multiscale and multiphenomena processes. There is a need for a multidisciplinary and system-oriented approach for the development of more generic models and simulation methods, achieved through the cross-fertilization of ideas across disciplines and the systematic flow of information among research groups. In addition, there is a need for the generic models and simulations developed to be made available to the nanoscale science and engineering community at large.

## II. PROGRAM DESCRIPTION

This initiative encourages team approaches to modeling and simulation of processes in nanostructures and nanosystems in the belief that a synergistic blend of expertise is needed to make major headway. Hence, this initiative has the aim of fostering a set of small interdisciplinary groups of experts (each made up of 3-5 principal investigators) that collaborate among themselves, augmented by collaboration across the set of funded groups to stimulate interactions among physical, mathematical, chemical, biological and engineering disciplines. This focused initiative will support research on new modeling and simulation methods and their extension and use to more than one discipline and one field across scales and phenomena. Ideally, the applicant groups will have established expertise in a field of nanoscale simulation research and are seeking the capability to collaborate with other groups to extend this knowledge to other fields of relevance and to understand the implications of multiphenomena/multiscale challenges on modeling and simulation methodologies, and to collaborate with industry. When funded, these groups will have the opportunity to develop their methodologies, and assess, compare and disseminate the results with the other research groups funded by this initiative and with the larger nanoscale modeling community funded by NSF and other agencies.

This initiative's focus is on high-risk/high-gain research areas leading to the development of synergistic collaborations, networking, and educational outcomes. Each group proposing is expected to:

- Address physical, mathematical, chemical and/or biological modeling and simulation techniques in the nanoscale range (about 1-100 nm). Examples include *ab initio* methods, quantum mechanics, molecular dynamics, grain and continuum-based models, stochastic methods, and nanomechanics;
- Carry out one or more of the following: Develop models and simulation techniques that embody multiscale and coupled multiphenomena, incorporate larger atomistic and molecular systems in models and simulations, advance outstanding theories such as nucleation and electron transport in order to significantly improve simulations, and/or take advantage of outstanding opportunities for development of theories and simulation methods by studying nanostructures;
- Extend existing models and simulation methods to formulations applicable to more than one discipline or field of application. Examples include coupled electrical and thermal processes and synthesis "by design" of nanostructures;
- Maintain continuous assessment of simulations on various aspects of nanoscience and engineering and seek opportunities for synergy with other groups. Each proposal must outline opportunities for the generalization of the proposed models and simulation methods. The results of the proposed work should be made available to the nanoscale science and engineering community via the web;
- Stimulate cross-disciplinary education through efforts such as the development of courses, short courses, software on the web, etc. and involve undergraduate and graduate students in the research;
- Collaborate with industry. Collaboration among universities, with national laboratories, and with centers of excellence in the U.S or abroad is encouraged, if appropriate for the proposed work.

This initiative is expected to lead to combined complementary strengths and synergism across the funded groups, exploratory research across the groups, new start-up research activities, and a shared data base and information on the Web available to the community at large. Additional information concerning related activities such as workshops and publications is available on-line at http://www.nsf.gov/nano.

## III. ELIGIBILITY INFORMATION

Proposals must be submitted by U.S. academic institutions with undergraduate and Ph.D. programs. Each group must have an engineering component. The proposers must show previously established, significant expertise and accomplishment in a discipline or field of relevance to modeling and simulation at the nanoscale. Principal investigators are required to form collaborations with industry, and the plan for industry/university interaction must be presented in the proposal. They may propose collaborations with government laboratories and centers of excellence in the U.S. or abroad, where appropriate. However, no NSF funds will be provided to support industry or government laboratories.

An institution (university or campus of a multi-campus university) may submit one proposal where only researchers from that institution are involved. The same institution may also submit

one other proposal as the lead institution in a multi-institution group proposal. That same institution may be a partner in any number of other multi-university group proposals in which it is not the lead. Group and collaborative proposals involving more than one institution must be submitted as a single administrative package from the lead institution. For these proposals, the lead university receives the funds from NSF and other sources and disburses them to the other partner institutions.

## IV. AWARD INFORMATION

Total award size per project is anticipated to be between $300,000 and $700,000 per year, depending upon the number of investigators, the nature of the research activity, and the availability of funds, with durations of up to three years. Three million dollars is allocated in FY 2000 for this initiative. A grantees' conference will review the progress of the projects and promote collaborations at the end of the first year, and at least one investigator from each project will be required to participate. This meeting will facilitate networking among the funded investigators and the development of a balanced and flexible infrastructure for nanoscale modeling and simulation in the U.S. The costs of attending this meeting should be included in the proposal budget.

## V. PROPOSAL PREPARATION & SUBMISSION INSTRUCTIONS

### A. Proposal Preparation Instructions.

Proposals submitted in response to this program solicitation should be prepared and submitted in accordance with the general guidelines contained in the *Grant Proposal Guide* (GPG), NSF 00-2. The plan for industry/university collaboration must be presented in the proposal. The complete text of the GPG (including electronic forms) is available electronically on the NSF Web site at: <http://www.nsf.gov/>. Paper copies of the GPG may be obtained from the NSF Publications Clearinghouse, telephone 301.947.2722 or by e-mail from pubs@nsf.gov.

Proposers are reminded to identify the program solicitation number (NSF 00-36) in the program announcement/solicitation block on the NSF Form 1207, "*Cover Sheet for Proposal to the National Science Foundation.*" Compliance with this requirement is critical to determining the relevant proposal processing guidelines. Failure to submit this information may delay processing.

### B. Budgetary Information – Cost Sharing Requirements.

None.

### C. Proposal Due Dates.

The proposal **MUST** be submitted by 5:00 PM, your local time, April 10, 2000 via FastLane. Detailed instructions for proposal preparation and submission via FastLane are available at https://www.fastlane.nsf.gov/a1/newstan.htm. Copies of the signed proposal cover sheet must be submitted in accordance with the instructions identified below.

*Submission of Signed Cover Sheets.* For proposals submitted electronically via FastLane, the signed proposal Cover Sheet (NSF Form 1207) should be forwarded to the following address within five working days following proposal submission in accordance with FastLane proposal preparation and submission instructions referenced above:

National Science Foundation
DIS-FastLane Cover Sheet
4201 Wilson Blvd.
Arlington, VA 22230

A proposal may not be processed until the complete proposal (including signed Cover Sheet) has been received by NSF.

### D. FastLane Requirements.

Proposers are required to prepare and submit all proposals for this Program Solicitation through the FastLane system. Detailed instructions for proposal preparation and submission via FastLane are available at: https://www.fastlane.nsf.gov/al/newstan.htm.

*Submission of Signed Cover Sheets.* The signed copy of the proposal Cover Sheet (NSF Form 1207) must be postmarked (or contain a legible proof of mailing date assigned by the carrier) within five days following proposal submission in accordance with the FastLane proposal preparation and submission instructions referenced above.

## VI. PROPOSAL REVIEW INFORMATION

### A. NSF Proposal Review Process.

Reviews of proposals submitted to NSF are solicited from peers with expertise in the substantive area of the proposed research or education project. These reviewers are selected by Program officers charged with the oversight of the review process. NSF invites the proposer to suggest, at the time of submission, the names of appropriate or inappropriate reviewers. Care is taken to ensure that reviewers have no conflicts with the proposer. Special efforts are made to recruit reviewers from non-academic institutions, minority serving institutions or adjacent disciplines to that principally addressed in the proposal.

Proposals will be reviewed against the following general merit review criteria established by the National Science Board. Following each criterion are potential considerations that the reviewer may employ in the evaluation. These are suggestions and not all will apply to any given proposal. Each reviewer will be asked to address only those that are relevant to the proposal and for which he/she is qualified to make judgments.

**What is the intellectual merit of the proposed activity?**

How important is the proposed activity to advancing knowledge and understanding within its own field or across different fields? How well qualified is the proposer (individual or team) to conduct the project? (If appropriate, the reviewer will comment on the quality of prior work.)

To what extent does the proposed activity suggest and explore creative and original concepts? How well conceived and organized is the proposed activity? Is there sufficient access to resources?

**What are the broader impacts of the proposed activity?**

How well does the activity advance discovery and understanding while promoting teaching, training, and learning? How well does the proposed activity broaden the participation of underrepresented groups (e.g., gender, ethnicity, disability, geographic, etc.)? To what extent will it enhance the infrastructure for research and education, such as facilities, instrumentation, networks, and partnerships? Will the results be disseminated broadly to enhance scientific and technological understanding? What may be the benefits of the proposed activity to society?

PIs should address the following elements in their proposal to provide reviewers with the information necessary to respond fully to both NSF merit review criteria. NSF staff will give these factors careful consideration in making funding decisions.

**Integration of Research and Education**

One of the principal strategies in support of NSF's goals is to foster integration of research and education through the programs, projects and activities it supports at academic and research institutions. These institutions provide abundant opportunities where individuals may concurrently assume responsibilities as researchers, educators, and students and where all can engage in joint efforts that infuse education with the excitement of discovery and enrich research through the diversity of learner perspectives.

**Integrating Diversity into NSF Programs, Projects, and Activities**

Broadening opportunities and enabling the participation of all citizens -- women and men, underrepresented minorities, and persons with disabilities -- are essential to the health and vitality of science and engineering. NSF is committed to this principle of diversity and deems it central to the programs, projects, and activities it considers and supports.

Proposals will be evaluated in accordance with the NSF merit review criteria described above and the additional criteria listed below.

- The level of expertise and accomplishment of the proposers in a discipline or field of relevance of modeling and simulation at the nanoscale;
- The potential of the proposed activity to enhance the interplay of multiphenomena at multiscales in different areas of nanoscale modeling and simulation;
- The degree to which the proposed activity will stimulate cross-disciplinary education through the development of curricula and the involvement of students in the research; and
- The strength of the plans for the required collaboration with industry.

Proposal review will be coordinated by a working group of NSF program officers. The selection process will involve a panel review to determine intrinsic merit and broad impact. Additional ad-hoc mail reviews may be used as well.

**B. Review Protocol and Associated Customer Service Standard**

All proposals are carefully reviewed by at least three academic, industrial or other government (non-NSF) experts in the particular field represented by the proposal. Proposals submitted in response to this solicitation will be reviewed by panels selected by the Nanoscale Modeling and Simulation Working Group.

Reviewers will be asked to formulate a recommendation to either support or decline each proposal. A program officer assigned to manage the proposal's review will consider the advice of reviewers and will formulate a recommendation. NSF will be able to tell applicants whether their proposals have been declined or recommended for funding within six months for 95 percent of proposals. The time interval begins on the proposal deadline or target date or from the date of receipt, if deadlines or target dates are not used by the program. The interval ends when the division director accepts the program officer's recommendation.

In all cases, after programmatic approval has been obtained, the proposals recommended for funding will be forwarded to the Division of Grants and Agreements for review of business, financial, and policy implications and the processing and issuance of a grant or other agreement. Proposers are cautioned that only a Grants Officer may make commitments, obligations or awards on behalf of NSF or authorize the expenditure of funds. No commitment on the part of NSF should be inferred from technical or budgetary discussions with an NSF Program officer. A principal investigator or organization that makes financial or personnel commitments in the absence of a grant or cooperative agreement signed by the NSF Grants Officer does so at its own risk.

## VII. AWARD ADMINISTRATION INFORMATION

**A. Notification of the Award.**

Notification of the award is made ***to the submitting organization*** by a Grants Officer in the Division of Grants and Agreements (DGA). Organizations whose proposals are declined will be advised as promptly as possible by the cognizant NSF Program Division administering the program. Verbatim copies of reviews, not including the identity of the reviewer, will be provided automatically to the Principal Investigator.

**B. Grant Award Conditions.**

An NSF grant consists of: (1) the award letter, which includes any special provisions applicable to the grant and any numbered amendments thereto; (2) the budget, which indicates the amounts, by categories of expense, on which NSF has based its support (or otherwise communicates any specific approvals or disapprovals of proposed expenditures); (3) the proposal referenced in the award letter; (4) the applicable grant conditions, such as Grant General Conditions (NSF GC-1)* or Federal Demonstration Partnership Phase III (FDP) Terms and Conditions* and (5) any NSF brochure, program guide, announcement or other NSF issuance that may be incorporated by reference in the award letter. Electronic mail notification is the preferred way to transmit NSF

grants to organizations that have electronic mail capabilities and have requested such notification from the Division of Grants and Agreements.

***** These documents may be accessed electronically on NSF's Web site at: <http://www.nsf.gov/>. Paper copies may be obtained from the NSF Publications Clearinghouse, telephone 301.947.2722 or by e-mail from pubs@nsf.gov.

More comprehensive information on NSF Award Conditions is contained in the NSF *Grant Policy Manual* (GPM) Chapter II, (NSF 95-26) available electronically on the NSF Web site. The GPM also is available in paper copy by subscription from the Superintendent of Documents, Government Printing Office, Washington, DC 20402. The GPM may be ordered through the GPO Web site at: <http://www.gpo.gov>. The telephone number at GPO for subscription information is 202.512.1800.

### C. Reporting Requirements.

For all multi-year grants (including both standard and continuing grants), the PI must submit an annual project report to the cognizant Program Officer at least 90 days before the end of the current budget period.

Within 90 days after expiration of a grant, the PI also is required to submit a final project report. Approximately 30 days before expiration, NSF will send a notice to remind the PI of the requirement to file the final project report. Failure to provide final technical reports delays NSF review and processing of pending proposals for that PI. PIs should examine the formats of the required reports in advance to assure availability of required data.

NSF has implemented a new electronic project reporting system, available through FastLane, which permits electronic submission and updating of project reports, including information on: project participants (individual and organizational); activities and findings; publications; and, other specific products and contributions. Reports will continue to be required annually and after the expiration of the grant, but PIs will not need to re-enter information previously provided, either with the proposal or in earlier updates using the electronic system.

## VIII. CONTACTS FOR ADDITIONAL INFORMATION

General inquiries should be made to any of the program directors listed in the "Cognizant Program Officers" section above. For questions related to use of FastLane, contact Ms. Esther Bolding, telephone (703) 306-1380, e-mail ebolding@nsf.gov.

## IX. OTHER PROGRAMS OF INTEREST

The NSF Guide to Programs is a compilation of funding for research and education in science, mathematics, and engineering. General descriptions of NSF programs, research areas, and eligibility information for proposal submission are provided in each chapter. Many NSF programs offer announcements concerning specific proposal requirements. To obtain additional information about these requirements, contact the appropriate NSF program offices listed in Appendix A of the GPG. Any changes in NSF's fiscal year programs occurring after press time

for the Guide to Programs will be announced in the NSF Bulletin, available monthly (except July and August), and in individual program announcements. The Bulletin is available electronically via the NSF Web Site at http://www.nsf.gov. The direct URL for recent issues of the Bulletin is http://www.nsf.gov/od/lpa/news/publicat/bulletin/bulletin.htm Subscribers can also sign up for NSF's Custom News Service to find out what funding opportunities are available.

## ABOUT THE NATIONAL SCIENCE FOUNDATION

The National Science Foundation (NSF) funds research and education in most fields of science and engineering. Grantees are wholly responsible for conducting their project activities and preparing the results for publication. Thus, the Foundation does not assume responsibility for such findings or their interpretation.

NSF welcomes proposals from all qualified scientists, engineers and educators. The Foundation strongly encourages women, minorities, and persons with disabilities to compete fully in its programs. In accordance with federal statutes, regulations, and NSF policies, no person on grounds of race, color, age, sex, national origin, or disability shall be excluded from participation in, be denied the benefits of, or be subjected to discrimination under any program or activity receiving financial assistance from NSF (unless otherwise specified in the eligibility requirements for a particular program).

Facilitation Awards for Scientists and Engineers with Disabilities (FASED) provide funding for special assistance or equipment to enable persons with disabilities (investigators and other staff, including student research assistants) to work on NSF-supported projects. See the program announcement or contact the program coordinator at (703) 306-1636.

The National Science Foundation has Telephonic Device for the Deaf (TDD) and Federal Information Relay Service (FIRS) capabilities that enable individuals with hearing impairments to communicate with the Foundation regarding NSF programs, employment, or general information. TDD may be accessed at (703) 306-0090 or through FIRS on 1-800-877-8339.

We want all of our communications to be clear and understandable. If you have suggestions on how we can improve this document or other NSF publications, please email us at plainlanguage@nsf.gov.

## PRIVACY ACT AND PUBLIC BURDEN STATEMENTS

The information requested on proposal forms and project reports is solicited under the authority of the National Science Foundation Act of 1950, as amended. The information on proposal forms will be used in connection with the selection of qualified proposals; project reports submitted by awardees will be used for program evaluation and reporting within the Executive Branch and to Congress. The information requested may be disclosed to qualified reviewers and staff assistants as part of the review process; to applicant institutions/grantees to provide or obtain data regarding the proposal review process, award decisions, or the administration of awards; to government contractors, experts, volunteers and researchers and educators as necessary to complete assigned work; to other government agencies needing information as part

of the review process or in order to coordinate programs; and to another Federal agency, court or party in a court or Federal administrative proceeding if the government is a party. Information about Principal Investigators may be added to the Reviewer file and used to select potential candidates to serve as peer reviewers or advisory committee members. See Systems of Records, NSF-50, "Principal Investigator/Proposal File and Associated Records," 63 Federal Register 267 (January 5, 1998), and NSF-51, "Reviewer/Proposal File and Associated Records," 63 Federal Register 268 (January 5, 1998). Submission of the information is voluntary. Failure to provide full and complete information, however, may reduce the possibility of receiving an award.

Public reporting burden for this collection of information is estimated to average 120 hours per response, including the time for reviewing instructions. Send comments regarding this burden estimate and any other aspect of this collection of information, including suggestions for reducing this burden, to: Reports Clearance Officer; Information Dissemination Branch, DAS; National Science Foundation; Arlington, VA 22230.

## YEAR 2000 REMINDER

In accordance with Important Notice No. 120 dated June 27, 1997, Subject: Year 2000 Computer Problem, NSF awardees are reminded of their responsibility to take appropriate actions to ensure that the NSF activity being supported is not adversely affected by the Year 2000 problem. Potentially affected items include: computer systems, databases, and equipment. The National Science Foundation should be notified if an awardee concludes that the Year 2000 will have a significant impact on its ability to carry out an NSF funded activity. Information concerning Year 2000 activities can be found on the NSF web site at http://www.nsf.gov/oirm/y2k/start.htm.

Catalogue of Federal Domestic Assistance (CFDA) No.: 47.041 – Engineering Grants
OMB No.: 3145-0058
NSF 00-36